

# Spontaneous and resonant lifting of the spin blockade in nanowire quantum dots

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A complete description of the dynamics of a two-electron system confined in narrow nanowire quantum dots under oscillating electric field and phonon mediated relaxation is presented in the context of recent electric dipole spin resonance experiments. We find that spin-orbit coupling results in lifting the spin blockade by spin non-conserving phonon mediated relaxation provided that the initial state is close in energy to the ground state which results in deblocking one of the Zeeman split triplets. At higher magnetic field, after singlet-triplet anticrossing new channel for lifting the Pauli blockade opens which results in an appearance of additional resonance lines, as present in recent experimental results [S. M. Frolov, et al., Phys. Rev. Lett. **109**, 236805 (2012)].

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In recent years gate defined nanowire [1] double quantum dots have been successfully used for experimental demonstration [2–8] of electrical control of single spins [9]. The spin rotations are performed by means of electric dipole spin resonance (EDSR) where spin-orbit (SO) interaction [10, 11] is used to electrically control the spin excluding the need for oscillating magnetic field in the device [12]. The spin oscillations are probed exploiting the spin blockade [13] of two-electron system where the current cycle  $(0, 1) \rightarrow (1, 1) \rightarrow (0, 2) \rightarrow (0, 1)$  [the numbers denote number of electrons in the adjacent quantum dots] is blocked at the  $(1, 1) \rightarrow (0, 2)$  transition when the spin configurations of the  $(1, 1)$  and  $(0, 2)$  states do not match. For low bias the only available  $(0, 2)$  state is the spin singlet so the current is blocked if the system is initialized in one of the spin-polarized triplets. The blockade is lifted when the spin of oscillating electron is rotated such the total spin of the  $(1, 1)$  state is changed from  $S = 1$  to  $S = 0$ . Relaxation of the  $(1, 1)$  state that follows the spin rotation opens the tunneling of the single electron through the double dot and is mediated by phonons that disperse the excess energy between the  $(1, 1)$  and  $(0, 2)$  states.

Strong SO coupling in InSb and InAs nanowires that is useful for effective control of the spins leads to spin relaxation [14–16] that results in lifting the spin blockade, limits the available magnetic fields for the EDSR [17] and results in the leakage current that exhibit dips or peaks at low magnetic field depending on the interdot coupling [18]. In the present Letter we study phonon mediated electron relaxation in electrically driven nanowire quantum dots. We find several unexpected features that are crucial for the mechanism of the spin blockade lifting: *i*) in all regions where the spin conserving  $(1, 1) \rightarrow (0, 2)$  relaxation occurs the spin non-conserving relaxation from  $(1, 1)$  triplet state with spins polarized along the magnetic field is of a very similar effectiveness. *ii*) For small magnetic fields where  $(0, 2)$  singlet is the ground state this leads to the spontaneous lifting of the spin blockade

from this triplet. *iii*) On the other hand the relaxation from triplet with spins oriented antiparallel to the magnetic field orientation is two orders of magnitude slower so the blockade is maintained. *iv*) At higher magnetic fields when the triplet becomes the ground state spin rotation accompanied by charge redistribution results in lifting spin blockade through direct transition to  $(0, 2)$  singlet which is visible in recent experimental maps [5].

The considered two-electron system is described by the Hamiltonian  $H(t) = \sum_i h^i(t) + e^2/(4\pi\epsilon\epsilon_0|\mathbf{r}_1 - \mathbf{r}_2|)$  where  $h^i(t)$  is single electron energy operator. For a narrow nanowire the charge occupies ground state of lateral quantization (here taken in the Gaussian form  $\psi(y, z) = (\sqrt{\pi}l)^{-1} \exp[-(y^2 + z^2)/2l^2]$ , with  $l = 20$  nm) which leads [19] to the two-electron Hamiltonian,

$$H_{1D}(t) = h_{1D}^1(t) + h_{1D}^2(t) + \frac{\sqrt{\pi/2}}{4\pi\epsilon_0\epsilon l} \operatorname{erfcx} \left[ \frac{|x_1 - x_2|}{\sqrt{2}l} \right], \quad (1)$$

with single-electron energy operator

$$h_{1D}(t) = \frac{\hbar^2 k_x^2}{2m^*} + V(x, t) - \alpha \sigma_y k_x + \frac{1}{2} \mu_B g(x) B \sigma_x, \quad (2)$$

where  $\hbar k_x = -i\hbar \nabla_x$  is momentum operator and  $H_{SO} = -\alpha \sigma_y k_x$  stands for Rashba SO coupling. We allow for position dependent  $g$ -factor in the device [2, 4, 5] and take  $g(x) = g[1 + \beta H(x)]$  where  $H(x)$  is Heavyside step function and  $\beta = 0.1$ . The potential is separated into  $V(x, t) = V_{QD}(x) + V'(x, t)$  where quantum dot confinement is described by  $V_{QD}(x) = V_c(x) + eF_{bias}x$ .  $V_c$  defines potential of two quantum dots of 138 nm width each separated by potential barrier of 25 nm width and 200 meV height. The driving AC electric field is assumed active in the left dot [2], so the time dependent part of the potential takes the form  $V'(x, t) = eF_{AC}x f(x) \sin(\omega_{AC}t)$  where  $f(x) = 1$  in the left dot and 0 outside – see the inset to Fig. 1(a).

We calculate eigenstates  $\Psi^n(x_1, \sigma_1, x_2, \sigma_2, t = 0)$  (with corresponding eigenenergies  $E^n$ ) of Hamiltonian Eq. (1) for  $t = 0$  and use them as

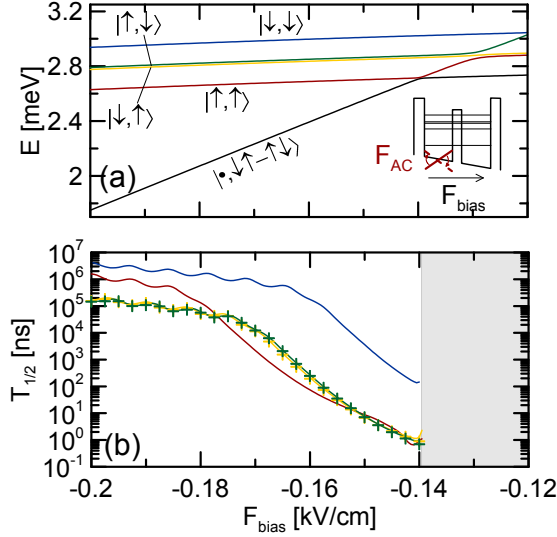


FIG. 1. (color online) (a) Energy levels of two-electron double quantum dot in function of bias electric field for  $B = 50$  mT. The arrows presents approximate spin polarization of electrons in the dots. The inset present schematics of the considered confinement potential. (b) Half-life time of excited states due to phonon mediated relaxation to the (0,2) singlet state. The colors of curves denote initial state of relaxation. The symbols (curves) corresponds to the results obtained without (with) SO interaction.

a basis for time evolution [20] where the two-electron spinor is expressed as  $\Psi(x_1, \sigma_1, x_2, \sigma_2, t) = \sum_n^N c_n(t) \exp(-iE_n t/\hbar) \Psi^n(x_1, \sigma_1, x_2, \sigma_2, t=0)$ .

To describe the phonon mediated relaxation we allow for the transitions between the two-electron states with rate given by the Fermi golden rule. The relaxation rate between the initial  $\Psi^i$  and final  $\Psi^f$  states is described by,

$$\tau_{if}^{-1} = \frac{2\pi}{\hbar} \sum_{\nu, i=1,2} \int_{\mathbf{q}} d\mathbf{q} |M_{\nu}(\mathbf{q})|^2 \times |\langle \Psi^f | e^{-i\mathbf{q}\mathbf{r}_i} | \Psi^i \rangle|^2 \delta(|E^f - E^i| - E_{\mathbf{q}}), \quad (3)$$

where the phonon dispersion relation is  $E_{\mathbf{q}} = \hbar c_{\nu} |\mathbf{q}|$  and  $c_{\nu}$  is the sound velocity. The sum in Eq. (3) goes over three types of electron-phonon scattering [20] due to: deformation potential with longitudinal mode ( $\nu = \text{LA-DP}$ ) [21], piezoelectric field ( $\nu = \text{LA-PZ}$ ) and piezoelectric field with transverse modes ( $\nu = \text{TA-PZ}$ ) [22].

The relaxation is included into time dependent calculation such the amplitude  $|c_n(t)|^2$  of each eigenstate is changed due to relaxation *to* all lower energy states and is increased due to relaxation *from* higher energy states with corresponding transition rates  $\tau_{if}$  [20]. This corresponds to 0K temperature where the energy instantly disperses and results in a half-life time of an  $i$ 'th state defined as  $T_{1/2} = \ln(2)/\tau_{if}$  due to relaxation to  $f$ 'th state.

We assume material parameters for InSb, i.e. electron effective mass  $m^* = 0.014$ ,  $g = -51$ , dielectric constant

$\varepsilon = 16.5$  and take the Rashba constant  $\alpha = 10$  meVnm. The AC field amplitude  $F_{AC} = 0.05$  kV/cm is assumed.

The charge distribution in the double dot is controlled by external voltages applied along the structure. Fig. 1(a) presents the lowest part of the energy spectrum (the subsequent energy levels – of (0,2) triplets – are above 5 meV) in function of bias electric field for  $B = 50$  mT. For the most negative values of  $F_{bias}$  the ground state is a singlet  $|\bullet, \downarrow \uparrow - \uparrow \downarrow\rangle$  state for which both electrons reside in the right dot [(0,2) configuration]. The four excited states correspond to single occupancy of each dot [(1,1) configuration] and energy of those states only weakly change in function of bias electric field. The two close in energy states, i.e.  $|\downarrow, \uparrow\rangle$  and  $|\uparrow, \downarrow\rangle$  correspond to definite and opposite spin configurations in each dot (i.e., in the  $|\downarrow, \uparrow\rangle$  state spin of the electron in the right dot – where the  $g$ -factor takes the highest value – is polarized along the magnetic field) resulting from mixing spin-zero triplet with singlet state by the  $g$ -factor mismatch between the dots. The two triplets  $|\uparrow, \uparrow\rangle$ ,  $|\downarrow, \downarrow\rangle$  are split by Zeeman interaction.

Let us inspect relaxation times of the four excited (1,1) states. In Fig. 1(b) we present half-life times of excited states due to relaxation to the ground state singlet. In the absence of SO interaction phonon scattering couples only states with the same total spin. Only the half-life times of  $|\uparrow, \downarrow\rangle$  and  $|\downarrow, \uparrow\rangle$  have finite values and they are presented with the crosses in Fig. 1(b). At low values of  $F_{bias}$  the times are of order of hundreds of microseconds but when the energy differences between the initial states and (0,2) singlet become lower the half-life times rapidly drop allowing for (1,1)  $\rightarrow$  (0,2) spin-conserving relaxation within nanoseconds for  $F_{bias} > -0.16$  kV/cm.

When SO coupling is included the spin polarization of the states becomes only approximate. The relaxation times of  $|\downarrow, \uparrow\rangle$  and  $|\uparrow, \downarrow\rangle$  states do not change – see the curves and crosses in Fig. 1(b). However now relaxation from all the (1,1) states to (0,2) singlet is open. For most negative values of  $F_{bias}$  half-life time of triplet states is longer than millisecond but when the bias field is increased the half-life time of  $|\uparrow, \uparrow\rangle$  triplet becomes about the same as the two spin opposite states lifting the spin blockade. Only the  $|\downarrow, \downarrow\rangle$  state remains effectively blocked with relaxation time longer by two orders of magnitude from the rest of the (1,1) states. This scenario was always repeated as we checked for different strengths of SO coupling and the dot size [20].

The experimental studies [7] report spin coherence time of order of tenths nanoseconds and coherent manipulation over a single spin up to 100 ns. We therefore focus on  $F_{bias}$  range where the relaxation times are of order of tenths of nanoseconds – hereafter we take  $F_{bias} = -0.15$  kV/cm – that allow for deblocking of single-electron current through the double dot after spin rotation in EDSR experiments. In Fig. 2(a) we plot energy levels in function of the magnetic field  $B$ . For  $B = 0$  the excited state

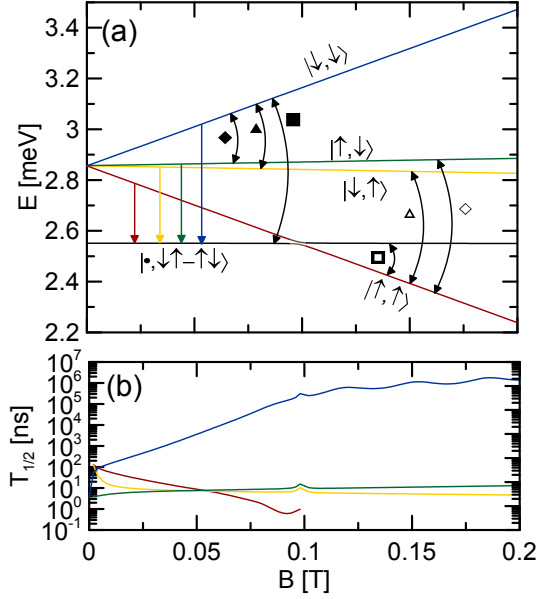


FIG. 2. (color online)(a) Energy spectrum in function of the magnetic field. Straight arrows denote transitions due to phonon relaxation. Curved arrows depict available EDSR resonances from the triplets. (b) Half-life time of excited states due to phonon mediated relaxation. Results obtained for  $F_{bias} = -0.15$  kV/cm.

is fourfold degenerate due to high interdot barrier – negligible exchange coupling. When the magnetic field is increased the energy levels of the two spin polarized triplets  $|\uparrow, \uparrow\rangle$  and  $|\downarrow, \downarrow\rangle$  are split by the Zeeman interaction. On the other hand the energy levels of the two spin-opposite states –  $|\downarrow, \uparrow\rangle$  and  $|\uparrow, \downarrow\rangle$  – are weakly split due to  $g$ -factor mismatch in the dots. At  $B = 0.1$  T an anticrossing between the energy levels of triplet  $|\uparrow, \uparrow\rangle$  and (0,2) singlet states appear followed by the change of the ground state.

Figure 2(b) presents half-life times of excited states due to relaxation to (0,2) singlet. We observe that the relaxation from spin antiparallel  $|\downarrow, \uparrow\rangle$  and  $|\uparrow, \downarrow\rangle$  states occurs within few nanoseconds regardless of  $B$  value. As the energy separation between energy levels of  $|\uparrow, \uparrow\rangle$  and (0,2) singlet decreases the relaxation time drops and after  $B = 50$  mT the half-life time of this state is even lower than the half-life time of spin-antiparallel states. On the other hand relaxation from  $|\downarrow, \downarrow\rangle$  state is slow and the half-life time grows for increasing magnetic field until  $B = 0.1$  T. This shows that for magnetic field range before the anticrossing only the  $|\downarrow, \downarrow\rangle$  triplet provides spin blockade as the  $|\uparrow, \uparrow\rangle$ ,  $|\downarrow, \uparrow\rangle$  and  $|\uparrow, \downarrow\rangle$  states decay quickly into  $|\bullet, \downarrow\uparrow - \uparrow\downarrow\rangle$ .

In EDSR experiments the two-electron system can initialize in any of the low energy states within the transport energy window. We therefore study the time evolution taking each of the (1,1) states with the energy levels depicted in Fig. 2(a) as an initial state. In Fig. 3(e)-(h) we present (0,2) occupation probability (which would allow

for tunneling of one of the electrons outside the dot lifting the blockade) averaged during 30 ns time evolution in function of the magnetic field and the electric field frequency.

For  $|\uparrow\uparrow\rangle$  taken as the initial state the probability is presented in Fig. 3(e). At the left part of the map we observe increasing probability in the background in function of  $B$  due to spin relaxation that results in spontaneous lifting of spin blockade. At  $B = 0.1$  T the phonon relaxation to singlet (0,2) from  $|\uparrow, \uparrow\rangle$  stops as the latter becomes the ground state – the background of the plot shows nearly zero (0,2) occupation probability. However we observe several resonance lines with increased probability. The resonance line ( $\Delta$ ) corresponds to the spin rotation in the left dot ( $|\uparrow, \uparrow\rangle \rightarrow |\downarrow, \uparrow\rangle$ ) accompanied by the phonon mediated relaxation to the  $|\bullet, \downarrow\uparrow - \uparrow\downarrow\rangle$  singlet which results in an increase of the (0,2) occupation probability – see Fig. 3(a) where we present the probability  $|c_n|^2$  of finding the system in the  $n$ 'th state during the time evolution. The ( $\diamond$ ) transition is related to the spin rotation in the right dot which is much less effective due to presence of the AC electric field only in the left dot and high interdot barrier which results in a narrow resonance line. The bottom line marked with ( $\square$ ) corresponds to the direct transition to the (0,2) singlet that involves charge reconfiguration between the dots – see Fig. 3(b). Note that line of increased probability due to  $|\uparrow, \uparrow\rangle \rightarrow |\bullet, \downarrow\uparrow - \uparrow\downarrow\rangle$  transition is not observed for  $B < 0.1$  T as in this region the spin relaxation of the triplet results in its fast deexcitation to the ground state with rate that exceeds the EDSR transition.

In Figs. 3(f), (g) one can observe mainly nonzero (0,2) occupation probabilities due to fast spin-conserving relaxation of  $|\downarrow, \uparrow\rangle$  and  $|\uparrow, \downarrow\rangle$  to the  $|\bullet, \downarrow\uparrow - \uparrow\downarrow\rangle$  state as discussed previously. In fact this relaxation is fast enough that one can observe lines of lowered probability when the system already relaxes into singlet (0,2) and is driven back to one of the excited states.

For the  $|\downarrow, \downarrow\rangle$  triplet taken as the initial state outside the resonances the (0,2) occupation probability is nearly zero at Fig. 3(h) as the phonon mediated relaxation from this state is slow – see the blue curve in Fig. 2(b). The lines that go through the diagonal of the plot – ( $\blacklozenge$ ), ( $\blacktriangle$ ) – corresponds to the transition to the  $|\downarrow, \uparrow\rangle$  and  $|\uparrow, \downarrow\rangle$  states respectively accompanied by relaxation to  $|\bullet, \downarrow\uparrow - \uparrow\downarrow\rangle$  [see Fig. 3(d)] and the line at the left upper part of the plot – ( $\blacksquare$ ) – is a direct transition to the (0,2) singlet that does not involve phonon mediated relaxation [see Fig. 3(c)].

Note that in maps of Fig. 3(a) and (d) also lines of increased probability at the half frequency of the ( $\square$ ) and ( $\blacksquare$ ) transitions are visible which is due to resonant harmonic generation by the driven electrons [23].

The experimentally [5] measured resonances at current maps are obtained from many sequential events of single electron transport through the structure. In each of them

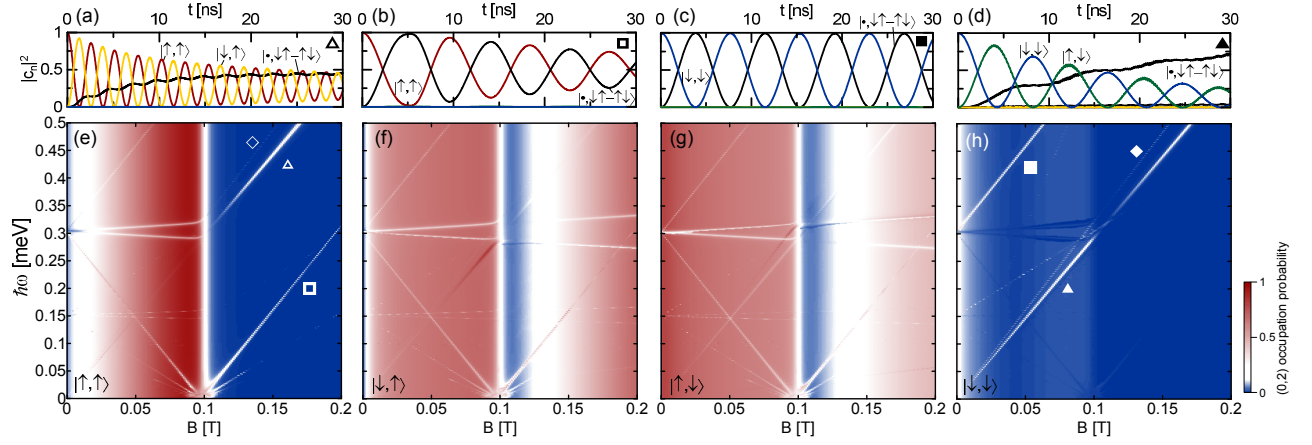


FIG. 3. (color online) (a)-(d) transitions between the eigenstates during the time evolution at the resonances marked with the symbols. (e)-(h) Probability of (0,2) occupation averaged during the 30 ns time evolution obtained for subsequent (1,1) states taken as the initial state of the time evolution – the spin configuration of the initial state is denoted in the left bottom corner of each plot.

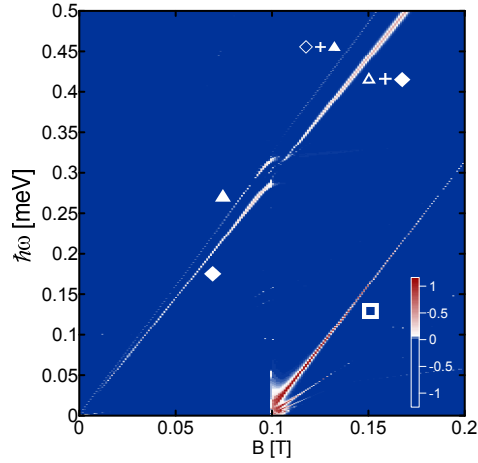


FIG. 4. (color online) Probability of (0,2) occupation averaged over the 30 ns time evolution calculated as a sum of results obtained for initial states with (1,1) occupation. For each  $B$  value the (0,2) occupation probability obtained for  $\hbar\omega_{AC} = 0$  (in the absence of driving electric field) was subtracted from the results.

the system can initialize in any of the (1,1) states. We therefore calculate the total probability of (0,2) occupation by summing the results for initial states presented in Figs. 3(e)-(h). For each value of  $B$  the probability obtained without (due to pure relaxation) the oscillating electric field is subtracted to mimic the experimental procedure of Ref. [5]. For low values of  $B$  we observe two lines at the diagonal of the map that corresponds to the transitions from  $|\uparrow, \uparrow\rangle$  state – rotation of the spin down to spin up in the left dot (bright line) or in the right dot (faint line) accompanied by relaxation to (0,2) singlet. After singlet-triplet anticrossing at  $B = 0.1$  T the lines correspond to transition from *both* the triplets. At  $B = 0.1$  T additional resonance line starts at the bottom

of the plot that corresponds to spin rotation with charge reconfiguration from  $|\uparrow, \uparrow\rangle$  triplet. Note that there is no similar line corresponding to transition from the  $|\downarrow, \downarrow\rangle$  state as it is compensated by the lowered probability obtained for evolution starting from  $|\downarrow, \uparrow\rangle$  and  $|\uparrow, \downarrow\rangle$ .

Similar arrangement of the resonance lines is preset in experimental map of Ref. [5] that probed wider range on magnetic field as compared with the previous experimental studies [2–4, 6, 7]. Especially the line that corresponds to ( $\square$ ) direct transition is visible which indicates the ground state change occurred blocking the low energy triplet state. One has to keep in mind however that in the experiment Ref. [5] the  $g$ -factor mismatch was compensated in some regions of the plot resulting in a single diagonal resonance line therein.

In conclusion we have presented the role that spin relaxation and EDSR plays on lifting the spin blockade in coupled nanowire quantum dots. We found that spin relaxation can lead to spontaneous lifting of the spin blockade such that the resonances are observed only from a single spin-blocked triplet state. The change of the ground state in higher magnetic fields leads to spin blockade of both the triplets and reveals additional resonance to the (0,2) singlet that do not involve phonon mediated relaxation and which is present in recent experimental results.

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